



Impact of interfacial charge transfer on the performance of Pd/C catalysts

Rao, Radhika G.; Blume, Raoul; Hansen, Thomas Willum; Fuentes, Erika; Dreyer, Kathleen; Hibbitts, David ; Chabal, Yves J.; Schloegl, Robert; Tessonnier , Jean Philippe

Publication date:
2017

Document Version
Peer reviewed version

[Link back to DTU Orbit](#)

Citation (APA):
Rao, R. G., Blume, R., Hansen, T. W., Fuentes, E., Dreyer, K., Hibbitts, D., Chabal, Y. J., Schloegl, R., & Tessonnier, J. P. (2017). *Impact of interfacial charge transfer on the performance of Pd/C catalysts*. Abstract from 254th National Meeting and Exposition of the American Chemical Society, Washington D.C., District of Columbia, United States.

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

ABSTRACT SYMPOSIUM NAME: Metal-Support Interactions in Catalysis: Modeling, Characterization & Design (Oral)

ABSTRACT SYMPOSIUM PROGRAM AREA NAME: CATL

CONTROL ID: 2750286

PRESENTATION TYPE: Oral Only : Do not consider for Sci-Mix

TITLE: Impact of interfacial charge transfer on the performance of Pd/C catalysts

AUTHORS (FIRST NAME, LAST NAME): Radhika G. Rao^{1, 2}, Raoul Blume³, Thomas W. Hansen⁴, Erika Fuentes⁵, Kathleen Dreyer⁶, David Hibbitts⁶, Yves J. Chabal⁵, Robert Schloegl³, Jean Philippe Tessonier^{1, 2}

INSTITUTIONS (ALL):

1. Chemical and Biological Engineering, Iowa State University, Ames, IA, United States.
2. NSF Engineering Research Center for Biorenewable Chemicals (CBIRC), Ames, IA, United States.
3. Max Planck Institute for Chemical Energy Conversion, Heterogeneous Reactions Group, Berlin, Germany.
4. Center for Electron Nanoscopy, Technical University of Denmark, Lyngby, Denmark.
5. Materials Science and Engineering and Physics, University of Texas Dallas, Richardson, TX, United States.
6. Department of Chemical Engineering, University of Florida, Gainesville, FL, United States.

ABSTRACT BODY:

Abstract: Carbon materials are typically considered to be inert catalyst supports. This assumption implies that carbon-supported catalysts are free of metal-support interactions. However, optoelectronic applications for nanocarbons demonstrate that their electronic properties can be tailored by varying their nanoscale structure and functionalization. This information suggests that the inertness of these materials for catalytic applications should be reconsidered as nanocarbons may be candidates for electronic metal-support interactions (EMSI).

In this work, we successfully decreased the structural complexity of carbon scaffolds and controlled their graphitization and surface functionalization. This approach enabled a detailed characterization of EMSI effects on Pd nanoparticles decorating these supports. Changes in selectivity for the hydrogenation of α,β -unsaturated aldehydes were observed when varying the support properties. The trends were free of artefacts such as differences in particle size, metal loading, and mass transfer effects. Detailed characterization of the catalysts using synchrotron based X-ray photoelectron spectroscopy and aberration corrected transmission electron microscopy confirmed the presence of electronic interactions between the Pd nanoparticles and carbon surface. Correlations were established between the extent of interfacial charge transfer, support properties, and catalyst selectivity. These experimental results were also confirmed using density functional theory calculations, providing stronger evidence for the presence of EMSI in Pd/C catalysts.

Our work demonstrates how the properties of carbon materials can influence the electronic structure of the supported metal active phase and thereby impact their catalytic performance. This study provides deeper insights into the tunability of EMSI effects and opens new avenues for the rational design of carbon-supported catalysts.

(No Image Selected)